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Time-dependent electron interference prior to ionization in the hydrogen atom and hydrogen molecular ion

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Synopsis We investigate electron dynamics in the hydrogen atom and the hydrogen molecular ion when exposed to long wavelength laser pulses yet having intensity insufficient to ionize the system. We find that the field is still able to drive the electron, leading to time-dependent interference effects.

In the literature, Strong Field Ionization theory often begins with the electron out of the system after tunnel ionization, but little is known about the dynamics within the system before ionization. In this poster we investigate electron dynamics in atoms and molecules for long wavelength laser pulses during the pulse rise but before an intensity high enough to ionize the system is reached. We compare the behaviour of the electron in the hydrogen atom with that in the hydrogen molecular ion.

Such studies require the solution of the Time-Dependent Schrödinger Equation (TDSE). The use of linearly polarised laser pulses aligned parallel to the internuclear axis of the molecular ion allows for the reduction of the problem to only two electronic spatial coordinates. It is appropriate to cast the problem in cylindrical polar co-ordinates. To this end we use a code that implements a combination of a finite difference method with a Lagrange mesh technique [1, 2]. The latter is a basis set method, which is based on Lagrange interpolation and Gaussian quadrature.

We subject the results of our calculations to scientific visualization analysis, first for the hydrogen atom and then for the hydrogen molecular ion. For H_2^+ we have performed two types of calculations. In the first type we assume the fixed-nuclei approximation. In the second, we partially lift this restriction by allowing internu-

clear quantum vibration along the fixed internuclear axis.

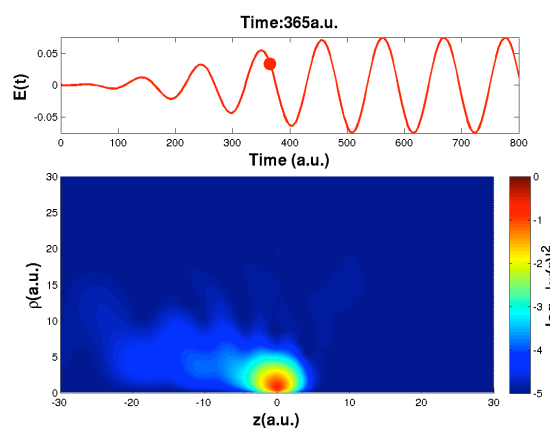


Figure 1. Cylindrical plot of the probability distribution function for the hydrogen atom, exposed to a laser pulse of $\lambda = 780$ nm and an intensity of $I = 2 \times 10^{14}$ W/cm². The pulse ramp on occurs over 5 optical cycles. The laser profile is given in the upper frame, where the position of the red circle represents the specific time of the calculation.

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References

- [1] D. Dundas 2002 *Phys. Rev. A* **65** 023408
- [2] D. Dundas, K.J. Meharg, J.F. McCann, K.T. Taylor 2003 *Eur. Phys. J. D* **26** 51

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